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Elastic scattering of electrons from methane molecule

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Abstract : Here we present our theoretical results for the differential scattering cross section and spin polarization parameters for elastic scattering of electrons from methane molecule at 100.00 eV using relativistic Dirac equation. The calculated spin polarization parameters are compared with those for iso-electronic neon and atomic carbon. The calculated angular distribution is compared with available experimental data.

Keywords : Elastic scattering, relativistic Dirac eqs., spin polarization

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1. Introduction

The recent technical advances in the study of the scattering of spin-dependent electrons have made it possible to understand the role of spin-dependent interactions in electron-atom collisions [1-3]. However, little work has been done on the related problem of spin polarization of electrons scattered from molecular systems. It is only in recent years that a few simple as well as sophisticated theoretical calculations of cross sections and spin polarization parameters of electron elastically scattered from oriented and simple diatomic molecules appeared [4-7].

Electron scattering from methane is of significant interest in many atmospheric and technological applications. CH_4 is one of the major greenhouse gases and also is an important constituent in the atmosphere of Jupiter, Saturn and our own planet. Theoretically and experimentally, electron collision with methane is very well studied problem. In recent years, considerable work has been done for cross sections and spin polarization of electrons scattered from methane molecule.

Various models have been used for these calculations. Here we are using a simple spherical complex optical potential (SCOP) approach along with the relativistic Dirac equation for calculating the spin polarization and cross sections for spherical molecules. It is well known that Dirac equation includes intrinsically the spin-orbit interaction along with other relativistic corrections. This approach has been quite successful in predicting the spin polarization parameters and cross sections of electrons elastically scattered from heavier atomic systems and polyatomic molecules like germane (GeH_4) and silane (SiH_4) [4].

In this paper, we are presenting our results for the scattering of electrons from methane molecule using the relativistic form of Schrödinger equation. The differential cross sections and the spin polarization parameters P, T and U are presented here only at 100 eV. To compare our results, we have also calculated the above scattering parameters for the atomic neon, isoelectronic to methane molecule, and the carbon atom.

2. Theoretical Methodology

In this calculation the motion of the projectile electron in a central field $V(r)$ is described by the Dirac equation

$$\left[c\vec{\alpha}.\vec{p} + \beta m_0 c^2 - V(r)\right]\Psi = E\Psi \qquad (1)$$

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For central potential, Dirac equation can be reduced to a set of two equations

$$g_l^{\pm''} + \left[K^2 - \frac{l(l+1)}{r^2} - U_l^{\pm}(r)\right] g_l^{\pm}(r) = 0 \qquad (2)$$

Where $g_l^{\pm}$ is related to the radial part $G_l^{\pm}$ of the large component of Ψ by

$$G_l = \sqrt{\eta}\frac{g_l}{r},$$

$$\eta = \frac{\left[E - V(r) + m_0c^2\right]}{c\hbar}$$

$$K^2 = \frac{E^2 - m_0^2c^4}{c^2\hbar^2}$$

Here, we take the total energy of the incident particle as $E = m_0\gamma c^2 = E_i + m_0c^2$, $\gamma = \left(1 - v^2/c^2\right)^{-\frac{1}{2}}$ where E_i as the kinetic energy of the incident particle of rest mass m_0 and velocity v. The $U_l^{\pm}$ are the effective Dirac potentials and are given in atomic units ($m_0 = e = \hbar = 1$, $1/c = \alpha$, where α is fine structure constant) as

$$-U_l^{\pm}(r) = -2\gamma V(r) + \alpha^2 V^2(r) - \frac{3}{4}\frac{(\eta')^2}{\eta^2} + \frac{1}{2}\frac{\eta}{\eta} \pm \binom{l+1}{l}\frac{1}{r}\frac{\eta''}{\eta} \qquad (3)$$

The single and double prime denotes the first and second order derivatives with respect to r.

Here, the total interaction between an electron and the target molecule is approximately represented by an effective potential, which can be expanded around the heavy central atom (carbon) in terms of a symmetry-adapted function of the A_1 irreducible representation (totally symmetric)

$$V_{eff}(r) = \sum_{l,h} V_{lh}(r) X_{lh}^{A_1}(\bar{r}) \qquad (4)$$

Retaining only the first term (with $l = 0$ and $h = 1$) in the expansion of Eq. (4), the spherical potential is written as

$$V_R(r) = V_{st}(r) + V_{ex}(r) + V_{pol}(r) \qquad (5)$$

The static potential $V_{st}(r)$ and charge density $\rho(r)$ are obtained using non-relativistic multicentre molecular wavefunction at the Hartree-Fock (HF) level, being generated from standard Quantum Chemistry computer codes. The molecular wavefunction are generated at experimental geometrices. The details are given in paper of Jain [8]. For the polarization potential we have used a parameter free polarization potential (V_{pol}), which is based on the correlation energy of the target atom. It has two components. The short range $V_{SR}(r)$ and long range $V_{LR}(r)$ parts and is given by

$$V_{pol}(r) = \begin{cases} V_{SR}(r) & r < r_c \\ V_{LR}(r) & r \geq r_c \end{cases}$$

r_c being the crossing point. The short-range part of polarization potential is given as

$$V_{SR}(r) = \begin{cases} 0.0311\ln r_s - 0.0584 + 0.006 r_s \ln r_s - 0.015 r_s, & r_s \leq 0.7 \\ -0.07356 + 0.02224\ln r_s & 0.7 < r_s \leq 10 \\ -0.584 r_s^{-1} + 1.988 r_s^{-3/2} - 2.45 r_s^{2} - 0.733 r_s^{5/2} & 10 < r_s \end{cases} \qquad (6)$$

where $r_s = [3/4\pi\rho(r)]^{1/3}$ and $\rho(r)$ is the electron charge density of the target system, but for the short range term for atomic systems are taken from the paper of Connell and Lane [9]. For exchange potential (V_{ex}), we have used the modified semi-classical exchange (MSCE) potential given by Gianturco and Scialla [10].

The impact energy range considered in the present calculation exceeds the threshold energy of the inelastic electrons scattering from the target systems under investigation and hence causes an absorption in the scattered beam. There exist various versions of the absorption potential describing all the inelastic processes during the scattering. To include the absorption effect in the scattered beam, we have therefore employed a modified version 3 of the semi-empirical model absorption potential of Staszewska *et al* [11]. It is given by

$$V_A = \frac{-1}{2} v_{loc}\rho(r)\bar{\sigma}_b \qquad (7)$$

$$v_{loc} = \left[2(E - V_R)\right]^{1/2} \qquad (8)$$

In Eqs. (7) and (8) v_{loc} is the local velocity of the incident electron for $E - V_R \geq 0$, v_R is the real part of the total interaction potential. The factor ½ in Eq. (7) is introduced to account for the exchange of the incident electron and bound electrons of the target during the scattering process. $\bar{\sigma}_b$ is the average quasifree binary collision cross section obtained non-empirically by using the free-electron gas model for the target. We avoid repeating the expressions, which are given in the paper of Staszewska *et al* [11]. The details of numerical calculations and the basic formulae to compute the various scattering and polarization parameters can be found in our previous paper [12].

3. Results and Discussions

In figure 1(a)–1(d), we have presented our DCS and spin polarization parameters P, T, U at 100 eV for electron elastically scattered from methane molecule. For comparison

with DCS and spin polarization (P) for methane molecule, we have also included the DCS and spin polarization for atomic iso-electronic neon (Ne) as well as for atomic carbon (C). In this figure we see, the general trend of variation of both DCS and spin polarization parameter (P) is quite similar for

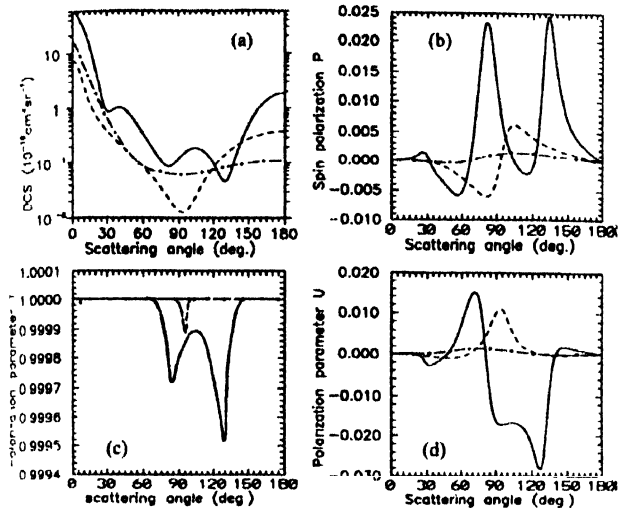

Figure 1a. Differential cross section for the scattering of electrons from the methane molecule (CH_4), carbon (C) and neon (Ne) atoms in units of 10^{-16} cm^2 sr^{-1} at 100.0 eV.

Present calculation ———CH_4; — • —C; - - - - Ne; (b) Spin polarization parameter P for electrons scattered from CH_4, C and Ne at 100 eV, (c) Spin polarization parameter T, (d) Spin polarization parameter U

each of the system except that position of the dip for neon atom, an iso-electronic system is shifted to larger angles. The additional broad peaks seen in the molecular curves at

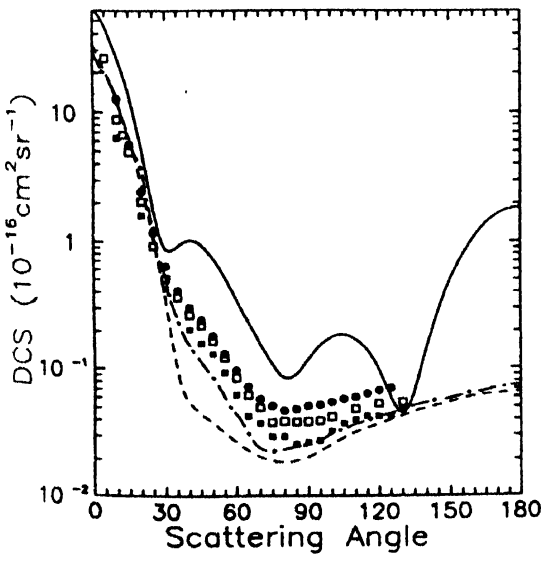

Figure 2. Differential cross section for the scattering of electrons from the methane molecule (CH_4) in units of 10^{-16} cm^2 sr^{-1} at 100.0 eV.

———Present result; - - - - A. Jain [8]; — • — • — Iga *et al* (theoretical) [13]; ••• Iga *et al* (Experimental) [13]; ■■ Boesten and Tanaka [14]. □□ Sakae *et al* [15].

higher angles show the presence of hydrogen (hydrogen bonds). The polarization function for carbon atom mimic simpler behaviour to that of methane but giving a very small value of polarization in the scattered beam behaving as a weak scatter.

Furthermore we also display our DCS curve in Figure 2 at 100 eV using the present relativistic model calculations together with other theoretical [8, 13] and experimental results [13-15]. It is found that, our DCS in this relativistic model reproduces the shape of DCS well but differs by an order of magnitude compared to the experimental data and with other theoretical calculations.

4. Conclusions

In summary, we report our results of relativistic calculations for DCS and spin polarization parameters, for the methane molecule at 100.00 eV within an optical potential approach. The calculated DCS reproduce the angular shape and size of the experimentally measured results within an order of magnitude. The neglect of the angular symmetry in the present interaction appears to be well justified, as the target molecule remains spherical for the incoming electron.

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